Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2024 – 04:23 PM JST

PDB ID	:	8XAC
Title	:	Crystal structure of amidase from Pseudonocardia acaciae
Authors	:	Takenoya, M.; Yajima, S.
Deposited on	:	2023-12-03
Resolution	:	3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

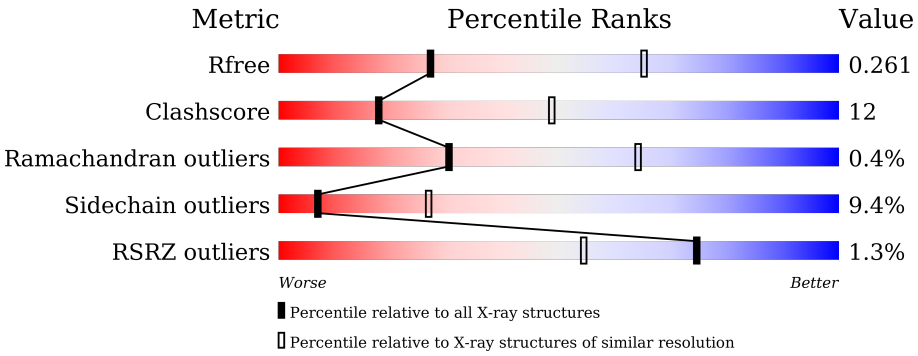
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	71% 25% • •
1	B	467	72% 24% • •
1	C	467	% 70% 24% • •
1	D	467	4% 56% 36% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Amidase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3392	2124	615	639	14			
1	B	456	Total	C	N	O	S	0	0	0
			3392	2124	615	639	14			
1	C	454	Total	C	N	O	S	0	0	0
			3377	2113	613	637	14			
1	D	455	Total	C	N	O	S	0	0	0
			3384	2118	614	638	14			

- Molecule 2 is water.

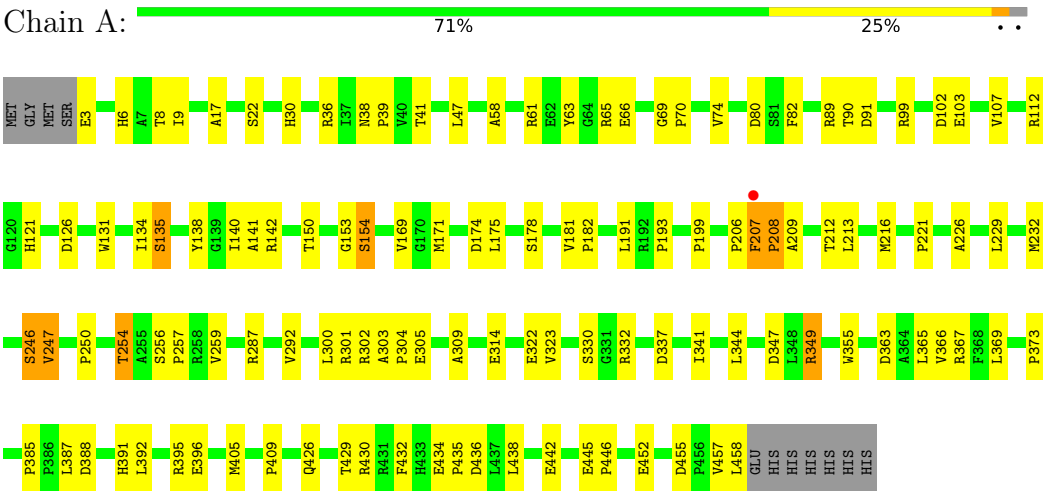
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	18	Total	O	0	0
			18	18		
2	C	15	Total	O	0	0
			15	15		
2	D	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

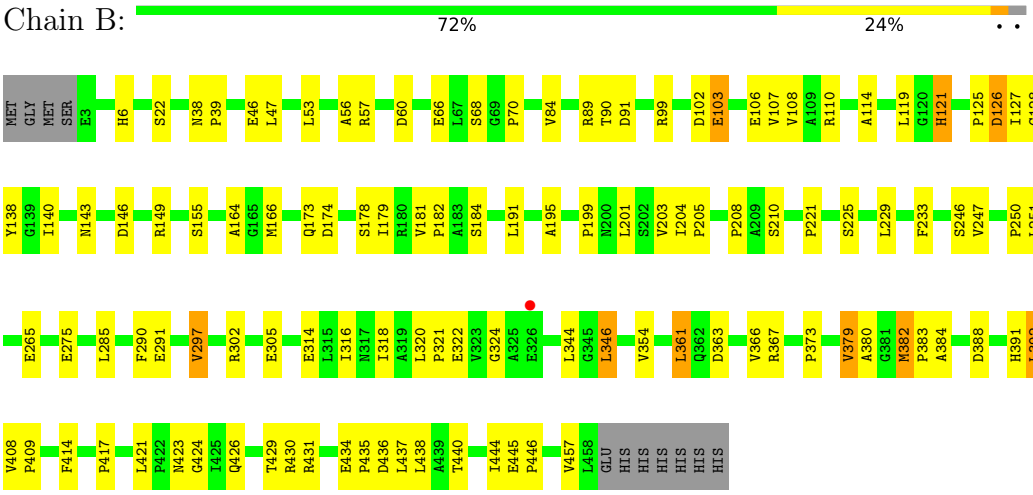
• Molecule 1: Amidase family protein

Chain A:



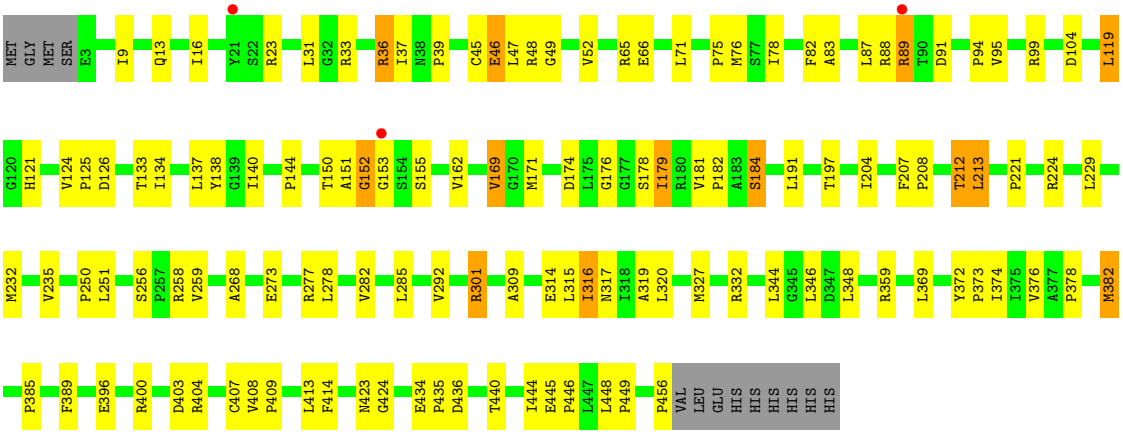
• Molecule 1: Amidase family protein

Chain B:



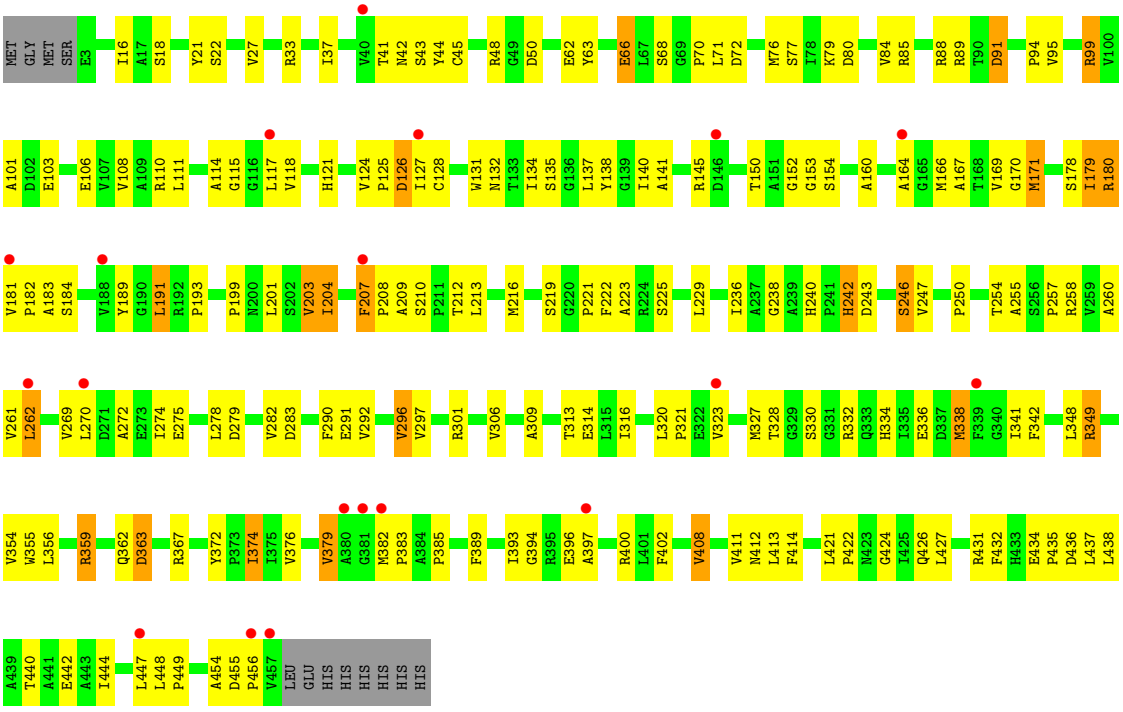
• Molecule 1: Amidase family protein

Chain C:



• Molecule 1: Amidase family protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	165.28Å 165.28Å 160.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.12 – 3.02 44.12 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.12-3.02) 99.8 (44.12-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.202 , 0.259 0.207 , 0.261	Depositor DCC
R_{free} test set	1946 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -l,-k,-h 0.000 for -h,-l,-k 0.000 for -h,l,k 0.012 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13607	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3465	0.72	0/4730
1	B	0.33	0/3465	0.67	0/4730
1	C	0.33	0/3450	0.66	0/4709
1	D	0.32	0/3457	0.65	0/4719
All	All	0.33	0/13837	0.68	0/18888

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3392	0	3358	76	0
1	B	3392	0	3358	65	0
1	C	3377	0	3338	79	0
1	D	3384	0	3347	114	0
2	A	26	0	0	2	0
2	B	18	0	0	0	0
2	C	15	0	0	1	0
2	D	3	0	0	0	0
All	All	13607	0	13401	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:HB2	1:C:179:ILE:HG23	1.51	0.91
1:C:184:SER:HB3	1:C:424:GLY:HA2	1.50	0.91
1:A:131:TRP:HA	1:A:153:GLY:HA3	1.55	0.89
1:D:181:VAL:HG23	1:D:408:VAL:HG11	1.62	0.82
1:A:131:TRP:HA	1:A:153:GLY:CA	2.10	0.81
1:C:36:ARG:O	1:C:39:PRO:HD2	1.80	0.81
1:D:33:ARG:HG3	1:D:37:ILE:HD13	1.63	0.80
1:D:262:LEU:HD12	1:D:297:VAL:HG11	1.68	0.76
1:C:89:ARG:CZ	1:C:204:ILE:HB	2.17	0.75
1:C:320:LEU:HD22	1:C:332:ARG:HD2	1.70	0.74
1:D:125:PRO:CD	1:D:154:SER:HA	2.19	0.73
1:B:429:THR:HG22	1:B:430:ARG:H	1.54	0.71
1:A:429:THR:HG22	1:A:430:ARG:H	1.54	0.71
1:D:221:PRO:HG2	1:D:229:LEU:HD22	1.73	0.71
1:D:394:GLY:O	1:D:397:ALA:HB3	1.92	0.69
1:D:44:TYR:OH	1:D:167:ALA:HB2	1.92	0.69
1:C:320:LEU:HD23	1:C:327:MET:HE1	1.75	0.69
1:C:153:GLY:HA3	1:C:182:PRO:HG3	1.76	0.68
1:D:43:SER:HB3	1:D:160:ALA:HB3	1.74	0.68
1:C:436:ASP:O	1:C:440:THR:HG23	1.94	0.67
1:D:208:PRO:O	1:D:213:LEU:HD21	1.95	0.67
1:D:152:GLY:HA3	1:D:182:PRO:HB3	1.76	0.67
1:A:221:PRO:HG2	1:A:229:LEU:HD22	1.76	0.67
1:C:212:THR:HG21	1:C:314:GLU:OE2	1.95	0.67
1:A:142:ARG:HG2	1:A:387:LEU:HD11	1.75	0.66
1:C:94:PRO:HA	1:C:137:LEU:HD13	1.76	0.66
1:B:125:PRO:HG2	1:B:128:CYS:HA	1.78	0.66
1:C:259:VAL:CG1	1:C:376:VAL:HG23	2.26	0.65
1:B:164:ALA:HB3	1:B:166:MET:HE2	1.78	0.65
1:D:212:THR:HG21	1:D:314:GLU:OE1	1.97	0.65
1:A:212:THR:HG22	1:A:355:TRP:HZ2	1.61	0.65
1:B:250:PRO:HD3	1:D:250:PRO:HD3	1.77	0.65
1:C:309:ALA:HB1	1:C:344:LEU:HD11	1.78	0.64
1:A:254:THR:HG22	1:A:436:ASP:OD2	1.97	0.64
1:D:125:PRO:HD2	1:D:154:SER:HA	1.80	0.64
1:A:254:THR:HG23	1:A:257:PRO:HG3	1.79	0.64
1:B:134:ILE:HG23	1:B:140:ILE:HG12	1.81	0.63
1:C:75:PRO:HB3	1:C:119:LEU:HD13	1.79	0.63
1:C:89:ARG:HB2	1:C:89:ARG:HH11	1.66	0.61
1:D:145:ARG:HH11	1:D:454:ALA:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HG22	1:D:108:VAL:HG11	1.82	0.61
1:A:169:VAL:HG11	1:A:232:MET:SD	2.41	0.61
1:B:285:LEU:HG	1:B:444:ILE:HD12	1.83	0.60
1:C:89:ARG:CD	2:C:510:HOH:O	2.49	0.60
1:C:221:PRO:HG2	1:C:229:LEU:HD22	1.84	0.60
1:D:106:GLU:HG3	1:D:110:ARG:HD2	1.82	0.60
1:A:80:ASP:O	1:A:89:ARG:HD2	1.99	0.60
1:D:154:SER:HB2	1:D:178:SER:HB3	1.83	0.60
1:D:180:ARG:HH12	1:D:411:VAL:HG21	1.66	0.60
1:D:91:ASP:O	1:D:126:ASP:O	2.20	0.59
1:D:131:TRP:HA	1:D:153:GLY:CA	2.32	0.59
1:C:445:GLU:HB3	1:C:446:PRO:HD3	1.85	0.59
1:A:322:GLU:HG3	1:A:323:VAL:HG13	1.84	0.59
1:D:272:ALA:HA	1:D:275:GLU:HB2	1.83	0.59
1:A:174:ASP:HA	1:A:178:SER:HB2	1.85	0.59
1:A:154:SER:HB2	1:A:178:SER:HB3	1.85	0.59
1:D:306:VAL:HG13	1:D:354:VAL:HG22	1.84	0.58
1:D:201:LEU:HD11	1:D:243:ASP:HB2	1.85	0.58
1:D:444:ILE:HB	1:D:448:LEU:HD13	1.85	0.58
1:D:131:TRP:HA	1:D:153:GLY:HA3	1.86	0.58
1:B:149:ARG:NH1	1:B:384:ALA:O	2.35	0.58
1:D:359:ARG:O	1:D:363:ASP:HB2	2.03	0.58
1:B:181:VAL:HB	1:B:182:PRO:HD3	1.86	0.57
1:A:341:ILE:HG12	1:A:395:ARG:HD2	1.86	0.57
1:A:379:VAL:HG22	1:A:426:GLN:HB3	1.86	0.57
1:D:282:VAL:HG13	1:D:292:VAL:HG11	1.85	0.57
1:C:285:LEU:CD1	1:C:376:VAL:HG21	2.35	0.56
1:B:174:ASP:HA	1:B:178:SER:HB2	1.86	0.56
1:B:436:ASP:O	1:B:440:THR:HG23	2.05	0.56
1:A:36:ARG:NH1	1:A:455:ASP:OD2	2.39	0.56
1:A:91:ASP:O	1:A:126:ASP:O	2.25	0.55
1:B:361:LEU:HB3	1:B:414:PHE:CZ	2.42	0.55
1:A:134:ILE:HG23	1:A:140:ILE:HG12	1.89	0.55
1:B:221:PRO:HG2	1:B:229:LEU:HD22	1.88	0.54
1:D:79:LYS:HZ1	1:D:154:SER:HB3	1.72	0.54
1:D:45:CYS:HB2	1:D:138:TYR:CE1	2.43	0.54
1:D:191:LEU:HB3	1:D:221:PRO:HD2	1.90	0.54
1:B:258:ARG:HG3	1:B:291:GLU:HB3	1.89	0.54
1:D:212:THR:HG22	1:D:355:TRP:HZ2	1.72	0.54
1:C:76:MET:HG2	1:C:169:VAL:HG12	1.91	0.53
1:C:316:ILE:HA	1:C:320:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:MET:HA	1:D:412:ASN:O	2.08	0.53
1:A:131:TRP:HA	1:A:153:GLY:HA2	1.89	0.52
1:B:344:LEU:HD11	1:B:354:VAL:HG11	1.90	0.52
1:C:258:ARG:HD2	1:C:372:TYR:CE1	2.43	0.52
1:A:391:HIS:CD2	1:A:392:LEU:HG	2.44	0.52
1:B:191:LEU:HB3	1:B:221:PRO:HD2	1.90	0.52
1:D:27:VAL:HG23	1:D:117:LEU:HD23	1.90	0.52
1:D:393:ILE:HG23	1:D:397:ALA:CB	2.38	0.52
1:D:37:ILE:HG21	1:D:164:ALA:HB1	1.91	0.52
1:D:189:TYR:HB2	1:D:223:ALA:O	2.10	0.52
1:A:70:PRO:HD2	1:A:114:ALA:HB1	1.91	0.52
1:A:63:TYR:HB3	1:A:66:GLU:O	2.09	0.52
1:C:282:VAL:HG13	1:C:292:VAL:HG11	1.91	0.52
1:C:369:LEU:O	1:C:373:PRO:HA	2.10	0.52
1:A:247:VAL:HG21	1:A:432:PHE:HZ	1.74	0.51
1:B:91:ASP:O	1:B:126:ASP:O	2.28	0.51
1:B:440:THR:O	1:B:444:ILE:HG22	2.09	0.51
1:D:124:VAL:O	1:D:135:SER:HB2	2.10	0.51
1:D:63:TYR:O	1:D:66:GLU:HB2	2.10	0.51
1:A:41:THR:O	1:A:141:ALA:HA	2.11	0.51
1:B:373:PRO:O	1:B:429:THR:HG23	2.11	0.51
1:A:153:GLY:O	1:A:178:SER:HA	2.11	0.51
1:D:71:LEU:O	1:D:115:GLY:O	2.29	0.51
1:A:309:ALA:HB1	1:A:344:LEU:HD11	1.93	0.50
1:B:184:SER:HB3	1:B:424:GLY:HA2	1.94	0.50
1:C:434:GLU:N	1:C:435:PRO:CD	2.74	0.50
1:D:76:MET:HG2	1:D:169:VAL:HG23	1.93	0.50
1:D:332:ARG:O	1:D:336:GLU:HG3	2.11	0.50
1:C:78:ILE:HG22	1:C:82:PHE:HB2	1.93	0.50
1:B:247:VAL:HG11	1:D:247:VAL:HG11	1.93	0.50
1:C:150:THR:HG21	1:C:389:PHE:CE1	2.46	0.50
1:C:259:VAL:HG11	1:C:376:VAL:HG23	1.94	0.50
1:B:361:LEU:HB3	1:B:414:PHE:HZ	1.76	0.50
1:C:71:LEU:HD21	1:C:232:MET:SD	2.51	0.50
1:C:181:VAL:HB	1:C:182:PRO:HD3	1.92	0.50
1:A:140:ILE:HG21	1:A:387:LEU:HD22	1.93	0.50
1:D:201:LEU:CD1	1:D:243:ASP:HB2	2.41	0.50
1:D:379:VAL:HG22	1:D:426:GLN:HE21	1.76	0.50
1:C:153:GLY:HA3	1:C:182:PRO:CG	2.42	0.50
1:C:278:LEU:O	1:C:282:VAL:HG23	2.12	0.50
1:D:37:ILE:HG23	1:D:456:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HD11	1:D:349:ARG:HD3	1.93	0.49
1:A:153:GLY:N	1:A:182:PRO:HG3	2.27	0.49
1:A:405:MET:O	1:A:409:PRO:HD3	2.11	0.49
1:B:247:VAL:HG11	1:D:247:VAL:CG1	2.42	0.49
1:C:89:ARG:HB2	1:C:89:ARG:NH1	2.26	0.49
1:D:258:ARG:HA	1:D:291:GLU:HG2	1.95	0.49
1:D:338:MET:HE1	1:D:402:PHE:HB2	1.95	0.49
1:B:391:HIS:CE1	1:B:392:LEU:HD23	2.48	0.49
1:D:260:ALA:HB2	1:D:372:TYR:CD2	2.48	0.49
1:D:201:LEU:HD21	1:D:242:HIS:HB2	1.94	0.49
1:D:374:ILE:HD12	1:D:437:LEU:HD23	1.95	0.49
1:D:164:ALA:HB3	1:D:166:MET:HE2	1.95	0.48
1:D:363:ASP:O	1:D:367:ARG:HG3	2.13	0.48
1:A:212:THR:HG21	1:A:314:GLU:OE2	2.13	0.48
1:C:83:ALA:HB2	1:C:89:ARG:HE	1.78	0.48
1:C:197:THR:HG23	1:C:251:LEU:HD21	1.95	0.48
1:B:70:PRO:HD2	1:B:114:ALA:HB1	1.94	0.48
1:B:445:GLU:HB3	1:B:446:PRO:HD3	1.94	0.48
1:A:250:PRO:HD3	1:C:250:PRO:HD3	1.96	0.48
1:B:127:ILE:HG23	1:B:129:ILE:HB	1.95	0.48
1:D:126:ASP:CG	1:D:328:THR:HG23	2.34	0.48
1:A:259:VAL:O	1:A:292:VAL:HA	2.13	0.48
1:C:378:PRO:O	1:C:407:CYS:HB3	2.14	0.48
1:A:36:ARG:HG2	1:A:457:VAL:HG21	1.96	0.48
1:D:254:THR:HG22	1:D:436:ASP:OD2	2.14	0.48
1:C:179:ILE:HD11	1:C:191:LEU:N	2.28	0.48
1:D:393:ILE:HG23	1:D:397:ALA:HB3	1.95	0.48
1:B:106:GLU:HB2	1:B:201:LEU:HB2	1.95	0.47
1:D:43:SER:HB3	1:D:160:ALA:CB	2.41	0.47
1:D:103:GLU:HB2	1:D:203:VAL:HG21	1.95	0.47
1:D:193:PRO:HG2	1:D:219:SER:O	2.13	0.47
1:A:126:ASP:OD1	1:A:135:SER:HA	2.15	0.47
1:C:48:ARG:HB3	1:C:87:LEU:HD21	1.96	0.47
1:C:259:VAL:HG12	1:C:376:VAL:HG23	1.96	0.47
1:C:46:GLU:OE2	1:C:88:ARG:HD2	2.15	0.47
1:C:448:LEU:HB3	1:C:449:PRO:CD	2.44	0.47
1:D:334:HIS:O	1:D:338:MET:HB2	2.15	0.47
1:D:400:ARG:HD2	1:D:400:ARG:HA	1.64	0.47
1:A:434:GLU:N	1:A:435:PRO:CD	2.78	0.47
1:C:89:ARG:NH1	1:C:204:ILE:HB	2.29	0.47
1:C:317:ASN:HB3	1:C:346:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:O	1:C:224:ARG:HD3	2.15	0.47
1:D:99:ARG:CD	1:D:204:ILE:HG21	2.45	0.47
1:C:169:VAL:HG11	1:C:232:MET:SD	2.55	0.47
1:D:216:MET:HG2	1:D:413:LEU:HA	1.97	0.47
1:C:171:MET:HE1	1:C:232:MET:CE	2.45	0.46
1:C:315:LEU:HA	1:C:319:ALA:HB3	1.97	0.46
1:D:152:GLY:HA3	1:D:182:PRO:CB	2.45	0.46
1:D:379:VAL:HG22	1:D:426:GLN:HB3	1.96	0.46
1:A:347:ASP:OD2	1:A:349:ARG:NH1	2.48	0.46
1:C:382:MET:HG2	1:C:404:ARG:HB3	1.97	0.46
1:B:290:PHE:CE1	1:B:440:THR:HG22	2.50	0.46
1:B:316:ILE:O	1:B:321:PRO:HD3	2.15	0.46
1:C:48:ARG:O	1:C:52:VAL:HG12	2.15	0.46
1:A:337:ASP:O	1:A:395:ARG:HD3	2.15	0.46
1:B:247:VAL:CG1	1:D:247:VAL:HG11	2.45	0.46
1:D:296:VAL:HG21	1:D:372:TYR:CE2	2.50	0.46
1:C:174:ASP:OD2	1:C:176:GLY:O	2.34	0.46
1:B:367:ARG:NH1	1:D:242:HIS:O	2.49	0.46
1:C:9:ILE:O	1:C:13:GLN:HB2	2.15	0.46
1:C:408:VAL:HG12	1:C:409:PRO:HD3	1.97	0.46
1:A:154:SER:CB	1:A:178:SER:HB3	2.45	0.46
1:C:144:PRO:HA	1:C:456:PRO:HG3	1.97	0.46
1:D:150:THR:HG21	1:D:385:PRO:HG2	1.98	0.45
1:A:90:THR:O	1:A:91:ASP:HB2	2.16	0.45
1:B:429:THR:HB	1:B:437:LEU:HD11	1.98	0.45
1:C:91:ASP:O	1:C:126:ASP:O	2.34	0.45
1:C:171:MET:HE1	1:C:232:MET:HE3	1.98	0.45
1:C:208:PRO:O	1:C:213:LEU:HD12	2.17	0.45
1:D:421:LEU:HB3	1:D:422:PRO:HD2	1.99	0.45
1:D:131:TRP:HA	1:D:153:GLY:HA2	1.98	0.45
1:A:153:GLY:O	1:A:154:SER:HB2	2.17	0.45
1:B:38:ASN:N	1:B:39:PRO:CD	2.80	0.45
1:B:320:LEU:O	1:B:324:GLY:HA3	2.17	0.45
1:D:183:ALA:HB2	1:D:222:PHE:HE1	1.79	0.45
1:D:338:MET:CE	1:D:402:PHE:HB2	2.46	0.45
1:B:46:GLU:O	1:B:121:HIS:N	2.45	0.45
1:D:434:GLU:N	1:D:435:PRO:CD	2.80	0.45
1:A:445:GLU:HB3	1:A:446:PRO:HD3	1.98	0.45
1:B:363:ASP:O	1:B:366:VAL:HG22	2.17	0.44
1:B:89:ARG:O	1:B:99:ARG:HD2	2.17	0.44
1:C:78:ILE:O	1:C:121:HIS:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:HG2	1:A:207:PHE:CD2	2.53	0.44
1:A:208:PRO:O	1:A:209:ALA:HB3	2.17	0.44
1:A:347:ASP:OD1	1:A:349:ARG:HB2	2.17	0.44
1:B:233:PHE:CE2	1:B:251:LEU:HD11	2.53	0.44
1:B:382:MET:HE2	1:B:382:MET:HB2	1.85	0.44
1:A:30:HIS:HB3	1:A:119:LEU:HD11	1.99	0.44
1:A:303:ALA:N	1:A:304:PRO:HD2	2.32	0.44
1:A:438:LEU:O	1:A:442:GLU:HG3	2.17	0.44
1:A:243:ASP:HB3	1:A:246:SER:HB2	2.00	0.44
1:B:103:GLU:HG3	1:B:203:VAL:HG11	1.99	0.44
1:D:382:MET:HG3	1:D:383:PRO:O	2.17	0.44
1:D:41:THR:O	1:D:141:ALA:HA	2.18	0.44
1:D:199:PRO:HD3	1:D:238:GLY:O	2.17	0.44
1:A:82:PHE:CE1	1:A:107:VAL:HG11	2.53	0.44
1:B:89:ARG:O	1:B:99:ARG:NH1	2.50	0.44
1:B:302:ARG:HD2	1:B:305:GLU:OE1	2.18	0.44
1:C:45:CYS:HB2	1:C:138:TYR:CZ	2.52	0.44
1:D:171:MET:HE3	1:D:236:ILE:HG21	2.00	0.44
1:B:90:THR:HG21	1:B:138:TYR:CE2	2.53	0.43
1:C:71:LEU:HD12	1:C:235:VAL:HG21	1.99	0.43
1:D:72:ASP:HA	1:D:115:GLY:HA3	2.00	0.43
1:A:171:MET:CE	1:A:232:MET:CE	2.95	0.43
1:A:256:SER:N	1:A:257:PRO:HD3	2.34	0.43
1:C:124:VAL:HG23	1:C:125:PRO:O	2.18	0.43
1:D:374:ILE:HD11	1:D:427:LEU:HD22	1.99	0.43
1:C:151:ALA:O	1:C:152:GLY:O	2.37	0.43
1:D:323:VAL:O	1:D:327:MET:HB2	2.19	0.43
1:A:191:LEU:O	1:A:193:PRO:HD3	2.19	0.43
1:A:247:VAL:HG21	1:A:432:PHE:CZ	2.51	0.43
1:B:53:LEU:O	1:B:57:ARG:HG3	2.19	0.43
1:D:334:HIS:NE2	1:D:338:MET:HG3	2.34	0.43
1:B:417:PRO:HD2	1:B:429:THR:O	2.18	0.43
1:D:362:GLN:HB2	1:D:414:PHE:CD1	2.53	0.43
1:D:431:ARG:O	1:D:432:PHE:HB2	2.17	0.43
1:A:302:ARG:HD2	1:A:305:GLU:OE1	2.19	0.43
1:A:363:ASP:O	1:A:367:ARG:HG3	2.17	0.43
1:A:226:ALA:HB3	1:A:442:GLU:HG2	2.01	0.43
1:A:150:THR:HG21	1:A:385:PRO:HG2	2.01	0.43
1:C:48:ARG:HD2	1:C:87:LEU:HD11	2.00	0.43
1:D:132:ASN:HB2	1:D:389:PHE:CE2	2.54	0.43
1:A:349:ARG:HD3	1:C:346:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:MET:O	1:B:409:PRO:HD3	2.18	0.42
1:C:413:LEU:HD23	1:C:414:PHE:CZ	2.54	0.42
1:B:208:PRO:HB3	1:D:356:LEU:HD21	2.02	0.42
1:A:17:ALA:O	1:A:65:ARG:HG2	2.19	0.42
1:B:90:THR:HG21	1:B:138:TYR:OH	2.18	0.42
1:B:434:GLU:HA	1:B:437:LEU:HD13	2.00	0.42
1:D:260:ALA:HB2	1:D:372:TYR:HD2	1.85	0.42
1:A:112:ARG:HG2	1:A:112:ARG:HH11	1.85	0.42
1:B:435:PRO:HA	1:B:438:LEU:HD12	2.02	0.42
1:C:155:SER:OG	1:C:178:SER:O	2.36	0.42
1:C:229:LEU:HD23	1:C:229:LEU:HA	1.85	0.42
1:D:70:PRO:HD2	1:D:114:ALA:HB1	2.02	0.42
1:D:79:LYS:HB2	1:D:171:MET:O	2.19	0.42
1:B:421:LEU:HB2	1:B:423:ASN:OD1	2.20	0.42
1:C:285:LEU:HD11	1:C:376:VAL:HG21	1.99	0.42
1:D:111:LEU:HD11	1:D:171:MET:CE	2.50	0.42
1:D:209:ALA:HA	1:D:213:LEU:HD11	2.01	0.42
1:D:240:HIS:ND1	1:D:242:HIS:HB2	2.34	0.42
1:A:171:MET:HE1	1:A:232:MET:HE3	2.02	0.42
1:B:314:GLU:HA	1:B:318:ILE:HD12	2.01	0.42
1:A:58:ALA:O	1:A:61:ARG:HB2	2.20	0.42
1:A:458:LEU:C	2:A:516:HOH:O	2.58	0.42
1:D:448:LEU:HB3	1:D:449:PRO:CD	2.49	0.42
1:B:195:ALA:O	1:B:431:ARG:HD3	2.19	0.42
1:D:316:ILE:O	1:D:321:PRO:HD3	2.19	0.42
1:A:134:ILE:HG12	1:A:140:ILE:HG23	2.01	0.41
1:D:184:SER:OG	1:D:424:GLY:HA2	2.19	0.41
1:D:438:LEU:O	1:D:442:GLU:HG3	2.19	0.41
1:B:110:ARG:NH2	1:B:199:PRO:HG3	2.35	0.41
1:C:45:CYS:HB2	1:C:138:TYR:CE1	2.55	0.41
1:D:243:ASP:O	1:D:246:SER:HB2	2.20	0.41
1:A:175:LEU:HD12	1:A:216:MET:HB2	2.02	0.41
1:A:363:ASP:HA	1:A:366:VAL:HG22	2.03	0.41
1:C:191:LEU:HB3	1:C:221:PRO:HD2	2.01	0.41
1:C:396:GLU:O	1:C:400:ARG:HD3	2.20	0.41
1:D:111:LEU:HD11	1:D:171:MET:HE2	2.02	0.41
1:D:127:ILE:HG23	1:D:327:MET:HG3	2.02	0.41
1:D:171:MET:CE	1:D:236:ILE:HG21	2.50	0.41
1:D:309:ALA:O	1:D:313:THR:OG1	2.25	0.41
1:C:285:LEU:CD2	1:C:444:ILE:HD11	2.50	0.41
1:D:393:ILE:HG23	1:D:397:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:MET:HE1	1:A:232:MET:CE	2.50	0.41
1:A:199:PRO:HD3	1:A:238:GLY:O	2.20	0.41
1:B:84:VAL:HG22	1:B:108:VAL:HG11	2.03	0.41
1:D:94:PRO:HA	1:D:137:LEU:HD13	2.02	0.41
1:D:179:ILE:HG12	1:D:222:PHE:CZ	2.55	0.41
1:B:56:ALA:O	1:B:60:ASP:N	2.48	0.41
1:D:320:LEU:N	1:D:321:PRO:CD	2.84	0.41
1:B:380:ALA:O	1:B:404:ARG:O	2.38	0.41
1:C:124:VAL:HA	1:C:133:THR:HG23	2.02	0.41
1:A:181:VAL:HB	1:A:182:PRO:HD3	2.02	0.41
1:A:369:LEU:O	1:A:373:PRO:HA	2.21	0.41
1:B:204:ILE:HA	1:B:205:PRO:HD3	1.94	0.41
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.95	0.41
1:B:383:PRO:O	1:B:384:ALA:C	2.59	0.41
1:C:301:ARG:HE	1:C:301:ARG:HB2	1.79	0.41
1:D:80:ASP:O	1:D:89:ARG:HD2	2.21	0.41
1:D:290:PHE:CZ	1:D:440:THR:HG22	2.56	0.41
1:A:9:ILE:HG23	1:A:74:VAL:HG21	2.02	0.41
1:C:385:PRO:HB2	1:C:389:PHE:HB3	2.03	0.41
1:D:150:THR:CG2	1:D:385:PRO:HG2	2.51	0.41
1:A:69:GLY:HA3	1:A:114:ALA:O	2.22	0.40
1:A:90:THR:HG21	1:A:138:TYR:OH	2.21	0.40
1:A:330:SER:HB2	2:A:519:HOH:O	2.20	0.40
1:B:143:ASN:HB3	1:B:146:ASP:O	2.21	0.40
1:C:23:ARG:NH2	1:C:66:GLU:O	2.55	0.40
1:D:255:ALA:C	1:D:257:PRO:HD3	2.42	0.40
1:A:38:ASN:N	1:A:39:PRO:CD	2.85	0.40
1:A:300:LEU:O	1:A:304:PRO:HD2	2.21	0.40
1:B:265:GLU:HG2	1:B:297:VAL:HB	2.02	0.40
1:D:85:ARG:HA	1:D:101:ALA:O	2.21	0.40
1:B:379:VAL:HG22	1:B:426:GLN:HB3	2.03	0.40
1:D:153:GLY:O	1:D:178:SER:HA	2.21	0.40
1:B:173:GLN:O	1:B:179:ILE:HG13	2.21	0.40
1:C:277:ARG:HD3	1:C:423:ASN:O	2.21	0.40
1:D:278:LEU:O	1:D:282:VAL:HG23	2.21	0.40
1:C:31:LEU:HD11	1:C:49:GLY:HA2	2.03	0.40
1:C:78:ILE:CG2	1:C:82:PHE:HB2	2.52	0.40
1:C:268:ALA:HA	1:C:403:ASP:O	2.22	0.40
1:D:77:SER:O	1:D:170:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/467 (97%)	439 (97%)	14 (3%)	1 (0%)	44	76
1	B	454/467 (97%)	435 (96%)	17 (4%)	2 (0%)	30	64
1	C	452/467 (97%)	425 (94%)	26 (6%)	1 (0%)	44	76
1	D	453/467 (97%)	409 (90%)	40 (9%)	4 (1%)	14	47
All	All	1813/1868 (97%)	1708 (94%)	97 (5%)	8 (0%)	30	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	203	VAL
1	D	379	VAL
1	A	208	PRO
1	B	322	GLU
1	D	68	SER
1	D	207	PHE
1	C	152	GLY
1	B	379	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/357 (97%)	322 (93%)	25 (7%)	12	38
1	B	347/357 (97%)	322 (93%)	25 (7%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	345/357 (97%)	317 (92%)	28 (8%)	9 33
1	D	346/357 (97%)	294 (85%)	52 (15%)	2 11
All	All	1385/1428 (97%)	1255 (91%)	130 (9%)	7 27

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	HIS
1	A	8	THR
1	A	22	SER
1	A	47	LEU
1	A	99	ARG
1	A	102	ASP
1	A	103	GLU
1	A	121	HIS
1	A	135	SER
1	A	154	SER
1	A	207	PHE
1	A	213	LEU
1	A	246	SER
1	A	247	VAL
1	A	254	THR
1	A	287	ARG
1	A	301	ARG
1	A	332	ARG
1	A	349	ARG
1	A	365	LEU
1	A	382	MET
1	A	388	ASP
1	A	396	GLU
1	A	452	GLU
1	B	6	HIS
1	B	22	SER
1	B	47	LEU
1	B	66	GLU
1	B	68	SER
1	B	102	ASP
1	B	103	GLU
1	B	107	VAL
1	B	119	LEU

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Mol	Chain	Res	Type
1	B	121	HIS
1	B	126	ASP
1	B	155	SER
1	B	210	SER
1	B	225	SER
1	B	246	SER
1	B	262	LEU
1	B	275	GLU
1	B	297	VAL
1	B	346	LEU
1	B	361	LEU
1	B	382	MET
1	B	388	ASP
1	B	392	LEU
1	B	408	VAL
1	B	457	VAL
1	C	16	ILE
1	C	33	ARG
1	C	36	ARG
1	C	37	ILE
1	C	46	GLU
1	C	47	LEU
1	C	65	ARG
1	C	89	ARG
1	C	95	VAL
1	C	99	ARG
1	C	104	ASP
1	C	119	LEU
1	C	134	ILE
1	C	140	ILE
1	C	169	VAL
1	C	179	ILE
1	C	184	SER
1	C	207	PHE
1	C	212	THR
1	C	213	LEU
1	C	256	SER
1	C	273	GLU
1	C	301	ARG
1	C	316	ILE
1	C	348	LEU
1	C	359	ARG

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Mol	Chain	Res	Type
1	C	374	ILE
1	C	382	MET
1	D	16	ILE
1	D	18	SER
1	D	21	TYR
1	D	22	SER
1	D	42	ASN
1	D	48	ARG
1	D	50	ASP
1	D	62	GLU
1	D	66	GLU
1	D	88	ARG
1	D	91	ASP
1	D	95	VAL
1	D	99	ARG
1	D	118	VAL
1	D	121	HIS
1	D	126	ASP
1	D	128	CYS
1	D	134	ILE
1	D	140	ILE
1	D	171	MET
1	D	179	ILE
1	D	180	ARG
1	D	191	LEU
1	D	204	ILE
1	D	207	PHE
1	D	210	SER
1	D	225	SER
1	D	242	HIS
1	D	246	SER
1	D	261	VAL
1	D	262	LEU
1	D	269	VAL
1	D	270	LEU
1	D	274	ILE
1	D	279	ASP
1	D	283	ASP
1	D	296	VAL
1	D	301	ARG
1	D	330	SER
1	D	338	MET

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Mol	Chain	Res	Type
1	D	341	ILE
1	D	342	PHE
1	D	348	LEU
1	D	349	ARG
1	D	359	ARG
1	D	363	ASP
1	D	374	ILE
1	D	376	VAL
1	D	396	GLU
1	D	408	VAL
1	D	447	LEU
1	D	455	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	HIS
1	B	433	HIS
1	C	51	GLN
1	C	96	HIS
1	D	391	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	456/467 (97%)	-0.47	1 (0%)	92	85	24, 37, 61, 115	0
1	B	456/467 (97%)	-0.24	1 (0%)	92	85	29, 47, 78, 95	0
1	C	454/467 (97%)	-0.19	3 (0%)	84	68	31, 50, 72, 110	0
1	D	455/467 (97%)	0.59	19 (4%)	41	24	42, 85, 107, 145	0
All	All	1821/1868 (97%)	-0.08	24 (1%)	74	54	24, 51, 96, 145	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	381	GLY	5.8
1	A	207	PHE	3.8
1	C	153	GLY	3.8
1	D	457	VAL	3.3
1	C	89	ARG	2.8
1	D	323	VAL	2.8
1	D	339	PHE	2.5
1	D	181	VAL	2.5
1	D	188	VAL	2.4
1	D	456	PRO	2.4
1	D	380	ALA	2.3
1	D	270	LEU	2.3
1	D	382	MET	2.3
1	D	146	ASP	2.2
1	B	326	GLU	2.2
1	D	117	LEU	2.2
1	D	127	ILE	2.2
1	D	40	VAL	2.1
1	D	164	ALA	2.1
1	D	207	PHE	2.1
1	D	447	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	2.1
1	C	21	TYR	2.0
1	D	397	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.